Benzene, 1-bromo-2-methyl-

Other names:	1-Bromo-2-methylbenzene
	1-Methyl-2-bromobenzene
	2-BROMOTOLUENE
	2-Bromo-1-methylbenzene
	2-Methylbromobenzene
	2-Tolyl bromide
	NSC 6532
	O-METHYLBROMOBENZENE
	O-TOLYLBROMIDE
	Toluene, o-bromo-
	o-Bromotoluene
	o-Methylphenyl bromide
	o-Tolyl bromide
	o-bromomethylbenzene
	toluene, 2-bromo-
Inchi:	InChI=1S/C7H7Br/c1-6-4-2-3-5-7(6)8/h2-5H,1H3
InchiKey:	QSSXJPIWXQTSIX-UHFFFAOYSA-N
Formula:	C7H7Br
SMILES:	Cc1ccccc1Br
Mol. weight [g/mol]:	171.03
CAS:	95-46-5

Physical Properties

Property code	Value	Unit	Source
affp	775.30	kJ/mol	NIST Webbook
basg	745.80	kJ/mol	NIST Webbook
gf	125.16	kJ/mol	Joback Method
hf	63.58	kJ/mol	Joback Method
hfus	12.82	kJ/mol	Joback Method
hvap	40.55	kJ/mol	Joback Method
ie	8.56 ± 0.03	eV	NIST Webbook
ie	8.60 ± 0.10	eV	NIST Webbook
ie	8.85	eV	NIST Webbook
ie	8.78 ± 0.01	eV	NIST Webbook
ie	8.53	eV	NIST Webbook
log10ws	-2.23		Aqueous Solubility Prediction Method

log10ws	-2.23		Estimated Solubility Method
logp	2.758		Crippen Method
mcvol	103.230	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
nfpah	%!d(float64=2)		KDB
pc	4414.96	kPa	Joback Method
rinpol	1022.72		NIST Webbook
rinpol	1012.00		NIST Webbook
rinpol	1037.00		NIST Webbook
rinpol	1037.00		NIST Webbook
rinpol	1042.66		NIST Webbook
rinpol	1016.90		NIST Webbook
rinpol	1029.00		NIST Webbook
rinpol	1053.73		NIST Webbook
rinpol	171.00		NIST Webbook
rinpol	1037.00		NIST Webbook
rinpol	1032.58		NIST Webbook
rinpol	1053.73		NIST Webbook
rinpol	1016.90		NIST Webbook
rinpol	1029.00		NIST Webbook
rinpol	1033.00		NIST Webbook
rinpol	1031.98		NIST Webbook
rinpol	1027.31		NIST Webbook
rinpol	1020.00		NIST Webbook
rinpol	171.00		NIST Webbook
ripol	1431.71		NIST Webbook
ripol	1449.23		NIST Webbook
ripol	1437.45		NIST Webbook
ripol	1483.00		NIST Webbook
ripol	1432.76		NIST Webbook
tb	454.15 ± 0.50	K	NIST Webbook
tb	454.90 ± 0.25	K	NIST Webbook
tb	454.90	K	NIST Webbook
tb	454.60 ± 0.50	K	NIST Webbook
tb	454.60 ± 0.50	K	NIST Webbook
tb	454.65 ± 0.40	K	NIST Webbook
tb	454.60 ± 0.50	K	NIST Webbook
tb	454.15	K	KDB
tb	454.55 ± 0.25	K	NIST Webbook
tb	454.60 ± 0.50	K	NIST Webbook
tc	691.11	K	Joback Method
tf	246.34 ± 0.06	K	NIST Webbook
tf	245.40 ± 0.02	K	NIST Webbook

tf	245.55	K	Aqueous Solubility Prediction Method
tf	245.05 ± 0.15	K	NIST Webbook
tf	246.55 ± 1.00	K	NIST Webbook
vc	0.382	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.84	J/mol×K	691.11	Joback Method
cpg	183.69	J/mol×K	496.33	Joback Method
cpg	193.39	J/mol×K	535.29	Joback Method
cpg	202.41	J/mol×K	574.24	Joback Method
cpg	210.80	J/mol×K	613.20	Joback Method
cpg	218.60	J/mol×K	652.15	Joback Method
cpg	173.28	J/mol×K	457.38	Joback Method
dvisc	0.0003720	Pa×s	425.72	Joback Method
dvisc	0.0004698	Pa×s	394.05	Joback Method
dvisc	0.0006180	Pa×s	362.38	Joback Method
dvisc	0.0008568	Pa×s	330.72	Joback Method
dvisc	0.0012729	Pa×s	299.06	Joback Method
dvisc	0.0003042	Pa×s	457.38	Joback Method
dvisc	0.0020771	Pa×s	267.39	Joback Method
hvapt	48.80	kJ/mol	310.50	NIST Webbook
hvapt	47.20	kJ/mol	388.50	NIST Webbook
hvapt	45.30	kJ/mol	435.50	NIST Webbook
hvapt	52.60	kJ/mol	376.00	NIST Webbook
pvap	0.08	kPa	287.20	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.07	kPa	285.20	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.21	kPa	302.20	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.25	kPa	305.20	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.30	kPa	308.20	Thermochemistry of Halogen-Substituted Methylbenzenes

pvap	0.30	kPa	308.20	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.30	kPa	308.20	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.29	kPa	308.20	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.39	kPa	313.10	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.40	kPa	313.10	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.39	kPa	313.10	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.39	kPa	313.10	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.39	kPa	313.10	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.39	kPa	313.10	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.06	kPa	284.20	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.05	kPa	281.20	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.14	kPa	296.20	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.11	kPa	293.20	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.09	kPa	290.20	Thermochemistry of Halogen-Substituted Methylbenzenes

pvap	0.08	kPa	287.20	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.17	kPa	299.20	Thermochemistry of Halogen-Substituted Methylbenzenes

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	332.20	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40569e+01
Coeff. B	-3.65275e+03
Coeff. C	-6.75980e+01
Temperature range (K), min.	332.88
Temperature range (K), max.	485.27

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.33837e+02
Coeff. B	-1.05118e+04
Coeff. C	-1.77738e+01
Coeff. D	1.43820e-05
Temperature range (K), min.	305.15
Temperature range (K), max.	385.15

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C95465&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1698.mol
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1698
Thermochemistry of Halogen-Substituted Methylbenzenes:	https://www.doi.org/10.1021/je500784s
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume